2-keto-13-epi-manoyl oxide

Inchi: InChI=1S/C20H32O2/c1-7-18(4)10-8-16-19(5)13-14(21)12-17(2,3)15(19)9-11-20(16,6)22
InchiKey: VYNOMUZYZAXYKN-UHFFFAOYSA-N
Formula: C20H32O2
SMILES: C=CC1(C)CCC2C(C)(CCC3C(C)(C)CC(=O)CC32C)O1
Mol. weight [g/mol]: 304.47

Physical Properties

Property code	Value	Unit	Source
gf	73.31	kJ/mol	Joback Method
hf	-412.86	kJ/mol	Joback Method
hfus	15.69	kJ/mol	Joback Method
hvap	63.27	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.922		Crippen Method
mcvol	263.220	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	2218.00		NIST Webbook
tb	776.97	K	Joback Method
tc	1028.96	K	Joback Method
tf	527.29	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	868.91	J/mol×K	776.97	Joback Method
cpg	898.17	J/mol×K	818.97	Joback Method
cpg	928.02	J/mol×K	860.97	Joback Method
cpg	959.05	J/mol×K	902.96	Joback Method
cpg	991.90	J/mol×K	944.96	Joback Method
cpg	1027.15	J/mol×K	986.96	Joback Method
cpg	1065.44	J/mol×K	1028.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R333445&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume